4. REVISIONS AND ADDITIONS TO TRIM.FaTE

Since May 1998, the Agency has implemented numerous revisions and additions to the TRIM.FaTE module, both in response to SAB comments (see Chapter 2) and as part of the ongoing model development. This chapter summarizes the major revisions and additions, including their basis and current status. As appropriate, revisions and additions to TRIM.FaTE will be assessed in the uncertainty and sensitivity analyses along with the model evaluation activities that are being conducted on this module. Technical terms used in this chapter are defined in the glossary (Appendix A) and in a text box at the beginning of Chapter 5. More detailed information on the aspects of the TRIM.FaTE module that are discussed below is presented in Volume I of the TRIM.FaTE TSD.

4.1 ABILITY TO ACCOUNT FOR METALS

Prior to May 1998, the chemical fate and transport algorithms developed for and included in TRIM.FaTE were specific to nonionic organic compounds, with phenanthrene and benzo(a)pyrene as the example chemicals for which all the necessary parameter values were obtained and used in the algorithms. The transfer coefficients used in these algorithms rely upon the concept of fugacity for modeling some types of chemical transfers; however, the concept of fugacity cannot generally be applied to metals and other inorganic compounds. Because addressing the impacts of metals and other inorganic compounds is a priority for OAQPS and to demonstrate that the TRIM.FaTE methodology is not restricted to modeling the fate and transport of organic compounds, algorithms have been added to TRIM.FaTE prototype V that address the fate and transport of inorganic compounds. The new algorithms were developed and included in TRIM.FaTE specifically for mercury and mercury compounds, but many of these algorithms can be used for other metals and inorganic compounds. Thus, TRIM.FaTE now has the flexibility to model fate and transport of organic and inorganic chemicals (assuming the chemical property values required as inputs are available or can be estimated).

4.2 ABILITY TO MODEL FATE AND TRANSPORT OF CHEMICAL TRANSFORMATION PRODUCTS

The transformation of chemical substances in the environment can have a profound effect on their potential for dispersion, persistence, accumulation, and exposure. Chemical transformations, which may occur as a result of biotic (*e.g.*, microbial degradation) or abiotic (*e.g.*, oxidation, hydrolysis) processes, can significantly reduce the concentration of a substance or alter its structure in such a way as to enhance or diminish its toxicity. For example, nitrogenous compounds, which are largely represented by aliphatic and aromatic amines, are of particular interest due to their potential genotoxic activities; transformation processes such as photolytic transformation and oxidation and reduction reactions can lead to the interconversion of these compounds between their related condensation products (*e.g.*, azo compounds) and oxidation products (*e.g.*, primary amines). Such transformations may prolong the persistence of these compounds in the environment and determine their genotoxic potencies (Layton et al. 1993).

Prior to May 1998, chemical transformation was represented in the TRIM.FaTE prototypes via the use of reaction sinks, and the fate of the transformed chemical was not tracked. That is, the mass of the chemical being transformed diminished over time, as appropriate, but the fate and transport of the newly created transformation product(s) was not tracked over time. Algorithms have been added to TRIM.FaTE prototype V to model reversible chemical transformation processes (*e.g.*, the transformation of elemental mercury (Hg) to divalent mercury (Hg^{2+}) and then back to elemental). These algorithms were developed specifically for three species of mercury (*i.e.*, elemental, divalent, methyl), although the general framework is applicable for any case in which first-order transformation is appropriate. This additional feature provides TRIM.FaTE with the ability to model the fate and transport of chemical transformation products, in addition to the disappearance of the chemical being transformed.

4.3 ABILITY TO ACCOUNT FOR SEASONALITY

Although few multimedia fate and transport models include seasonal components, these are desirable for two reasons: (1) for the model to be applicable to regions in the U.S. where below-freezing temperatures occur, and (2) for model runs with durations extending beyond a single growing season. However, model realism gained by accounting for seasonality must be balanced with the burden on the user to collect site-specific data. Therefore, only selected seasonal algorithms have been implemented in TRIM.FaTE at this time.[1]

Since May 1998, two principal seasonal components have been added to TRIM.FaTE: litterfall algorithms and plant uptake of chemicals. The algorithms that have been implemented reflect the seasonality in the following ways:

- During litterfall, which is assumed to be either continuous for one month or one year (depending on the vegetation type), the mass of chemical that is in and on the leaves is transferred to the surface soil compartments; and

- Uptake of chemicals by plants occurs only between the day of last and first frost.

A third seasonal process, harvesting (*i.e.*, removal of pollutant mass from the system), may be easy to implement in TRIM.FaTE; however, the module has not yet been tested in agricultural regions where this process would be relevant.

Additional seasonal processes may be considered in future improvements to TRIM.FaTE. In addition to evaluating the significance of the process to pollutant transfers among media within the modeling system (and the resultant media concentrations), an important part of this consideration will be the extent of modeling revisions needed for implementation in TRIM.FaTE. For example, some seasonal processes would require that the mass and volume of a compartment change during a model run (*e.g.*, growth dilution), and the current implementation of TRIM.FaTE does not include changes to compartment mass or volume with time. Methods may be devised to accommodate this, as in the case of litterfall, which as implemented in TRIM.FaTE does not

[1] Seasonal weather patterns are accounted for in the meteorological data inputs.

involve a change in the mass of the leaves within the compartment. Instead, for litterfall, uptake of the chemical ceases in the winter, and the chemical is transferred from the leaf compartments to the surface soil compartments.

Examples of seasonal processes that may affect pollutant distribution within the modeling system include the following.

- **The dynamics of snow.** The dynamics of snow accumulation and snowmelt and the timing of chemical transfers from snow to water may affect long-term chemical exposure estimates.

- **Growth of organisms.** The dilution of chemical concentrations in an organism because of its growth may affect predicted organism concentrations and dose rates.

- **Litterfall to surface water.** Litterfall to streams and lakes may affect the dynamics of chemical behavior in surface water.

- **Transformation of chemicals in litter.** The transformation of chemicals in leaf litter may occur at a different rate from that in surface and root zone soil; however, little information on these processes is available at this time.

- **Senescence of plant foliage.** Senescence of plant leaves can result in altered gas exchange with leaves, altered rates of chemical transformation in leaves, lowered water content of leaves, and altered uptake rates of chemicals from soil.

- **Blooming of algae.** The timing and rate of growth of algae, not incorporated in the current version of TRIM.FaTE, may affect the assumed exposure of aquatic organisms to chemicals. Furthermore, the sedimentation of algae following a bloom would affect the mass of a chemical in the sediment.

- **Dietary changes of wildlife.** Some wildlife species change diets at different times of the year, affecting chemical exposure estimates.

- **Habitat use.** Some wildlife species hibernate, winter sleep, or migrate from the contaminated region during winter. These seasonal differences in habitat use could decrease exposure to chemical contaminants.

- **Excretion periods.** Excretion of chemical body burdens by egg-laying and lactation occur during spring and summer seasons. These seasonal excretions may affect chemical body burdens and exposure levels of organisms.

4.4 OTHER ADDITIONS AND IMPROVEMENTS TO ALGORITHMS

This section highlights major changes and additions to the TRIM.FaTE algorithms. Detailed information on TRIM.FaTE algorithms is presented in Volume II of the TRIM.FaTE TSD.

4.4.1 ABIOTIC ALGORITHMS

The TRIM.FaTE module addresses chemical fate and transport within and between seven different abiotic compartment types (see adjacent text box). Many of the current abiotic algorithms were included in an earlier prototype of TRIM.FaTE. Since May 1997, however, several additions and improvements have been made.

ABIOTIC COMPARTMENT TYPES IN TRIM.FaTE

Air	Surface Water
Surface Soil	Sediment
Root Zone Soil	Ground Water
Vadose Zone Soil	

4.4.1.1 Dispersive Transport Between Surface Water Compartments

The current implementation of the TRIM.FaTE methodology retains the assumption that chemical mass is homogeneous within compartments. However, algorithms have been developed for addressing dispersive transport between surface water compartments (*i.e.*, surface water to surface water). This addresses a limitation of previous TRIM.FaTE prototypes because dispersion may be an important mechanism of transfer of some chemicals. In surface water compartments (see Chapter 4 of the TRIM.FaTE TSD Volume II), the algorithms are based on the methods used in the Water Quality Analysis Simulation Program (WASP) (Ambrose et al. 1995). Thus, TRIM.FaTE can now model the transport of chemicals by both dispersive and advective processes between surface water compartments.

4.4.1.2 Diffusion and Advection With Soil Compartments

During the last year, EPA developed a new approach for constructing air-to-soil and soil-to-soil chemical transport algorithms for TRIM.FaTE. This approach provides a simple but reliable method for simulating the transport of chemicals in soil. The new algorithm applies to three soil compartment types: (1) surface soil, (2) root zone soil, and (3) vadose zone soil. These different soils can be represented by two or more soil compartment types for the purpose of assessing chemical mass transfer. Two types of chemical transport are considered by the soil algorithm: (1) diffusion and (2) advection. The top soil layer (*i.e.*, surface soil compartment) exchanges chemical mass with the lowest compartment of the atmosphere (see Section 5.3.1.1) by a combination of diffusion and several advection processes – wet deposition, dry deposition, and resuspension. Each soil layer also can have one or more transformation processes. The specific links for soil compartments for which TRIM.FaTE includes algorithms are discussed in Chapter 5.

Quantifying the exchange of chemical mass between air and soil and among soil layers depends strongly on the concentration gradient within the soil layers. The Agency recognized

that any algorithm that properly addresses chemical mass transfer from air and into soil must account for the concentration gradient. Therefore, EPA developed an exact analytical solution by applying the appropriate boundary conditions to the transport/transformation equations as presented by Jury (1983). The Agency then developed a simplified form of this solution as the basis for an equivalent mass exchange algorithm that is applicable to each soil layer. Differential equations describing the dispersion, diffusion, advection, and transformation of chemicals distributed among air and soil layers were developed and solved analytically in one dimension. An evaluation of the mathematical behavior of the analytical solution resulted in the development of an approximate mathematical form, which uses a series of exponential functions to represent the variation of concentration with depth. Unlike the analytical solution, which requires fixed boundary conditions, these simple forms can be dynamically linked to other compartments in a multimedia fate model. The new algorithm makes it possible to calculate a characteristic soil penetration depth for each chemical based on the chemical's diffusion and degradation rates in various soil types. To confirm the accuracy of the simple model, several chemical property sets were used to compare results of the simple model against the analytical solution. The Agency only needed to conduct testing with a few chemical property sets because the equations are normalized for the chemical-specific soil penetration depth. Therefore, TRIM.FaTE can now be used to assess the penetration of chemicals from air into soil and provide results that are comparable to those obtained from more complex models. The current restriction on this approach is that the chemical concentration in air must be greater than the concentration in the gas phase of the vadose zone soil.

4.4.1.3 Diffusive Transport Between Surface Water and Sediment Compartments

Diffusive transport of chemicals between sediment and surface water compartments in both directions has been addressed in the current TRIM.FaTE prototype using standard methods as discussed in the Water Quality Analysis Simulation Program (WASP) (Ambrose et al. 1995). Inclusion of these algorithms in TRIM.FaTE is important because diffusive exchange of a chemical between surface water and sediment can be a primary means of transport for some chemicals. The methods adopted from WASP allow for the specification of a diffusive water flow velocity, allowing the movement of a chemical between sediment and sediment pore water in the dissolved phase to be simulated. Thus, TRIM.FaTE is capable of modeling the chemical transport between sediment and surface water compartments (in either direction), including sediment pore water.

4.4.2 BIOTIC ALGORITHMS

In addition to the abiotic compartment types and algorithms, the TRIM.FaTE module includes numerous biotic compartment types and algorithms related to terrestrial and aquatic plants and animals. The biotic algorithms in TRIM.FaTE represent chemical transfers to and from biotic and abiotic compartments, primarily through diffusion, advection, and dietary uptake processes (see Chapter 5 for additional information on biotic compartment types and algorithms).

Since May 1998, a number of changes and additions to the biotic algorithm library in TRIM.FaTE have been implemented, including the following:

- Several biotic algorithms were added to the library to estimate the accumulation of chemicals by new biotic compartment types, including algae, soil arthropods, plant foliage (as distinct from leaf surface), and plant leaf surfaces (as distinct from plant foliage);

- Minor improvements were made to several existing biotic algorithms, such as diffusion of chemicals into plant foliage, particle washoff from plant leaf surfaces, and litterfall;

- Several alternative biotic algorithms were added to the library to estimate the accumulation of chemicals by various biotic compartment types, including fish, plant roots, and earthworms; and

- An algorithm was added to the library to represent the link between plant stems and leaves.

4.4.3 CHEMICAL- OR CHEMICAL CLASS-SPECIFIC ALGORITHMS

Chemical- or chemical class-specific algorithms are included in TRIM.FaTE to model chemical fate and transport processes that are specific to a particular chemical or chemical class and that cannot be as accurately represented in the more generic abiotic or biotic algorithms. Because of the specificity of chemical- and chemical class-specific algorithms, the TRIM.FaTE module will be most useful and cost-effective if only a small number of chemical-specific algorithms are included (*i.e.*, if the algorithms included are applicable to a broad range of chemicals so new algorithms do not often have to be developed for new applications). At this time, a few chemical-specific biotic algorithms are necessary because certain chemical parameters (*e.g.*, rate constants, partition coefficients) are only applicable to certain chemicals and chemical classes. For example, biotic uptake of a specific chemical may be dependent on particular environmental parameters. The goal, however, is to implement generic algorithms for all important transport and transformation processes, supplemented by class-specific algorithms (*e.g.*, for metals) as needed, and to minimize the use of chemical-specific algorithms to chemicals and processes where a real benefit can be realized. In the current version of TRIM.FaTE, algorithms are included that (1) are applicable to high priority chemicals, such as mercury and polycyclic aromatic hydrocarbons (PAHs), (2) pose issues in multiple environmental media, and (3) are not addressed by other EPA models.

The previous prototype of TRIM.FaTE included some chemical class-specific algorithms for PAHs in support of the TRIM.FaTE test case. To test the ability of TRIM.FaTE to model metals, the Agency added some chemical-specific algorithms for mercury. For example, TRIM.FaTE now includes an algorithm to model the transformation of methylmercury to divalent mercury in plant leaves and stems. More detailed information on the mercury-specific algorithms included in the current prototype is presented in Appendix A of Volume II of the TRIM.FaTE TSD.

4.5 INTERFACE WITH EXTERNAL MODELS

Over the past year, the Agency developed and implemented methods for incorporating the results from an external fate and transport model (*e.g.*, an air model, such as ISCST3) within the current TRIM.FaTE framework. This provides additional flexibility because, for example, external model data can be used in place of certain TRIM.FaTE algorithms during a simulation. These methods are described in detail in Appendix B of the TRIM.FaTE TSD Volume I. These methods have been implemented in prototype V of TRIM.FaTE in two ways: (1) the results of an external air model (*e.g.*, ISCST3) can be used as input data, and (2) the concentration can be fixed in specified compartments during a simulation. In either case, certain TRIM.FaTE algorithms are bypassed and essentially "replaced" by model results or fixed concentrations.

As discussed in Appendix B of TRIM.FaTE TSD Volume I, there are limitations with this approach. Either the linkage between the model and TRIM.FaTE is in one direction only and, hence, conservation of chemical mass is lost, or the external model must be linked with TRIM.FaTE in such a way so that chemical transfer can occur in both directions. The difficulty of the latter option will depend on the particular external model considered, but it is likely that it would generally require a substantial effort to implement. This is because the user must not only perform the practical tasks associated with computer programming, but also must ensure that no fundamental assumptions or concepts inherent to either model are violated. Such a violation could occur, for example, if there is overlap between the models in how they address other processes that are not an explicit component of the model linkage itself (*e.g.*, the external model may be treating deposition using general inputs for vegetative cover, and the user must implement additional checks to ensure that these inputs are consistent with the vegetative compartments used within TRIM.FaTE).

The user guidance materials to be developed in the next TRIM development phase will caution users to carefully consider which external air models should be used as input to TRIM.FaTE. External models for various media can be used in lieu of the TRIM.FaTE algorithms; however, strong caution should be placed on the use of external models that themselves may not conserve mass (*e.g.*, Gaussian plume models), but whose use may be dictated or preferred for regulatory reasons.

4.6 METHODOLOGY FOR DETERMINING PARAMETERS OF THE MODELING ENVIRONMENT

While previous prototypes of TRIM.FaTE allowed for specification of the parameters of the modeling environment (*e.g.*, scale and spatial resolution, and selection of parcels, volume elements, and compartments), it did not provide a structured process for the user to follow. As a first step in designing this feature, the Agency has developed a consistent general stepwise procedure for setting up a simulation using TRIM.FaTE. These general steps are described in detail in Chapter 5 of TRIM.FaTE TSD Volume I and summarized below. Appendix C of TRIM.FaTE TSD Volume I provides, as an example, more detailed discussion for one step: defining the parcels used in setting up the spatial configuration of a model application.

1. **Define the analysis objective.** As part of the problem definition phase (*i.e.*, the first step in developing a TRIM.FaTE simulation), the user defines the objective of the analysis, including the chemical(s) of concern, the potentially exposed population(s), and the health and/or ecological effects endpoint(s) to be assessed.

2. **Define parcels.** The user considers factors including the likely pattern of transport and transformation of each chemical of concern (*i.e.*, where significant concentration gradients are likely to occur), the location of natural boundaries, and locations of key receptors to help determine the appropriate level of complexity (*e.g.*, size of modeling region, location, size, and number of parcels) for the simulation. The TRIM.FaTE module is intended for local-scale assessments of multimedia pollutant distribution.

> A **parcel** is a planar (*i.e.*, two-dimensional) geographical area used to subdivide a modeling region. Parcels, which can be virtually any size or shape, are the basis for defining volume elements. There can be air, land, and surface water parcels.

3. **Designate volume elements and compartments.** After parcels have been defined and boundaries established, the user designates volume elements and then defines abiotic and biotic compartments. Abiotic compartments include air, surface soil, root zone soil, vadose zone soil, surface water, sediment, and ground water. The depths of each abiotic compartment can be based on generic values, chemical-specific values (*e.g.*, whether a chemical is likely to penetrate deeply into the soil), or site-specific values (*e.g.*, the average depth of a modeled pond). The landscape property values assigned to compartments (*e.g.*, fraction organic carbon, amount of particles in the air) can be based on generic values or site-specific values. Biotic compartments include terrestrial and aquatic organisms; only plant compartments are required to be included in a simulation. A user can perform an assessment for an entire trophic group or for a particular animal species of concern.

4. **Select links and algorithms.** Following the establishment of TRIM.FaTE compartments for a given simulation, the appropriate links and algorithms are selected to model mass transfer and transformation. This step may include specifying the data or data source and the algorithms to use or may in some cases require a user to add algorithms to the algorithm library.

5. **Determine specifications for the simulation.** The last step of TRIM.FaTE setup is preparing the simulation, which involves specifying the simulation time-step, the chemical properties of each modeled chemical, the initial distribution of the chemical mass in the compartments, the data for each modeled source, all site data needed by the selected algorithms, and the output time period(s) of interest.

The steps above describe the general process for setting up a simulation using TRIM.FaTE. The flexible, user-friendly design of TRIM.FaTE provides the user with the ability to perform simulations in an iterative fashion. That is, the user is able to select the necessary level of analysis, ranging from a simple analysis, for which less site-specific data are required and which will run more quickly, to one needed for a more detailed risk assessment. For

example, the more simple analysis, providing a more imprecise, general idea of pollutant distribution, may be sufficient for setting priorities or other similar scoping activities (*e.g.*, in a screening analysis for which conservative default input parameters could be used). This allows the user to focus a more detailed analysis, where the impacts of parameter uncertainty may be assessed for critical parameters, on situations where a more refined assessment is needed (*e.g.*, human health risk assessments to support environmental regulation or other environmental control actions).

4.7 OVERVIEW OF THE UNCERTAINTY AND VARIABILITY ANALYSIS APPROACH SELECTED FOR TRIM

In accordance with National Academy of Sciences guidance (NRC 1994), current EPA risk characterization guidance (U.S. EPA 1995a, U.S. EPA 1995b), and updated guidance being developed (*e.g.*, U.S. EPA 1998c), EPA is developing TRIM to allow for stochastic modeling so that uncertainty and variability can be explicitly characterized. This involves the development of an approach to estimate uncertainty and variability within TRIM in a manner that allows for integration between the TRIM modules and for tracking the uncertainty and variability through the modules. At this time, an overall uncertainty and variability analysis approach has been developed for TRIM, as described in Chapter 3 of this report. Chapter 6 of TRIM.FaTE TSD Volume I describes the specific approach being implemented for TRIM.FaTE.

Following a review of current peer reviewed literature and assessment of the available options for uncertainty and variability analyses (see Appendix B), the Agency selected a staged approach for analysis of uncertainty and variability in TRIM, which has advantages for models as complex as TRIM. This approach provides the user with the option to include one of two stages of uncertainty and variability analyses in the simulation. The first stage, consisting of analyses that are comparatively easy to implement, identifies influential parameters and gives an importance-ranking of parameters. This information is useful for narrowing down the number of parameters to be analyzed in a more complex uncertainty and variability analysis. This first stage can be considered a sensitivity and screening analysis. The second stage involves uncertainty and variability analyses of increasing detail and complexity. For TRIM, a Monte Carlo approach was selected for this stage. This approach entails performing numerous model runs with model inputs randomly sampled from specified distributions for the model inputs. Figure 3-1 illustrates this staged approach for TRIM.FaTE.

As work on TRIM.FaTE and the other TRIM modules progresses, EPA plans to continue to evaluate new uncertainty analysis techniques for applicability to improving the current methodology. For example, methods using Fourier transforms, such as the Fourier Amplitude Sensitivity Test (Saltelli et al. 1999), will be evaluated in this context.

4.8 MODEL EVALUATION

In its May 1998 review, SAB recognized the challenge in developing a methodological framework for evaluating a model such as TRIM.FaTE. In developing the evaluation plan for TRIM.FaTE, the Agency has attempted to design an approach that contains the essential ingredients for judging the acceptability of TRIM.FaTE for its intended uses, while allowing enough flexibility to accommodate new methods that become available or changes in direction indicated by knowledge gained through the evaluation process. Chapter 6 presents a detailed description of the model evaluation plan designed for TRIM.FaTE.

The evaluation plan for TRIM.FaTE includes four types of model evaluation activities, described below.

- **Conceptual model evaluation** activities focus on whether the model is conceptually sound. This type of evaluation begins in the early stages of model development.

- **Mechanistic and data quality evaluation** activities focus on the algorithms and assumptions used in the model. They determine whether the individual process models and input data used are scientifically sound, and if they properly "fit together."

- **Structural evaluation** activities focus on how changes in modeling complexity affect model performance. They address, for example, the effects of varying the level of both temporal and spatial resolution.

- **Performance evaluation** activities focus on whether the output of the full model is relevant, reliable, and useful. They involve comparing modeling results to some type of benchmark (*e.g.*, monitoring data, other model results, expert judgment).

The first three types of evaluation focus primarily on model inputs (*e.g.*, theory and data) and processing (*e.g.*, process models, assumptions and algorithms, model setup), while the fourth focuses mainly on the information that comes out of the model (*e.g.*, comparing overall model outputs to environmental monitoring data).

The model evaluation plan designed for TRIM.FaTE must be flexible. Results from initial evaluation efforts are posing new questions and leading to additional review, analysis, and testing. A number of evaluation activities have been completed or are underway (*e.g.*, code verification, model documentation, peer review, case studies, sensitivity analysis), while others are still in the conceptual or planning stages.